

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.28e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.80e-01

Confidence level: 3.38e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Methylcyclopentane</div> <div>Measured: 9.75e-11</div> <div>Predicted: 80.1</div>	<div>Image not found</div> <div>Hydroprene</div> <div>Measured: 3.39e-09</div> <div>Predicted: 8.80e-04</div>	<div>Image not found</div> <div>2,3-Benzofluorene</div> <div>Measured: 1.35e-04</div> <div>Predicted: 2.22e-07</div>
<div>Image not found</div> <div>Fluorene</div> <div>Measured: 7.50e-07</div> <div>Predicted: 9.71e-04</div>	<div>Image not found</div> <div>Triphenylene</div> <div>Measured: 2.08e-05</div> <div>Predicted: 1.87e-08</div>	